

=> d his

(FILE 'HOME' ENTERED AT 06:34:18 ON 25 NOV 2002)  
FILE 'CA' ENTERED AT 06:34:30 ON 25 NOV 2002  
L1 2373516 S MIXTURE OR MIXED OR MIXING OR MIX  
L2 99211 S DATABASE OR DATA BASE OR LIBRARY  
L3 584065 S STANDARD OR CALIBRAT?  
L4 4213 S L1 AND L2  
L5 75121 S L1 AND L3  
L6 391 S L4 AND L5  
L7 2488078 S GRAPH? OR MODEL? OR DISPLAY? OR REPRESENT? OR DIAGRAM  
L8 444110 S L7 AND (TEMP OR TEMPERATURE OR DEG)  
L9 73451 S L1-3 AND L8  
L10 33 S L6 AND L9  
L11 141 S L6 AND (LIQUID OR FLUID OR SOLUTION OR AQUEOUS OR WATER OR H<sub>2</sub>O)  
L12 139476 S TITRATE# OR TITRANT OR TITRATION OR TITRATING  
L13 178081 S L1(3A) (PREPAR? OR FORM? OR MAKE)  
L14 16857 S L1(5A) (PLURAL? OR MULTI? OR ARRAY OR LIBRARY)  
L15 1306 S L13 AND L14  
L16 9 S L12 AND L15  
L17 552 S L15 AND (LIQUID OR FLUID OR SOLUTION OR AQUEOUS OR WATER OR H<sub>2</sub>O)  
L18 48 S L17 AND (REPLAC? OR REMOV?)  
L19 15 S L17 AND L3  
L20 34 S L8 AND L17  
L21 51852 S L1 AND REFERENCE NOT L5  
L22 369 S L4 AND L21  
L23 20 S L22 AND L8  
L24 112 S L22 AND (LIQUID OR FLUID OR SOLUTION OR AQUEOUS OR WATER OR H<sub>2</sub>O)  
L25 381 S L10-11, L16, L18-20, L23-24  
L26 252 S L25 NOT PY>1998  
L27 4 S L25 AND PATENT/DT NOT L26 AND PY<1999  
L28 256 S L26-27

=> d bib,ab 1-256 128

L28 ANSWER 23 OF 256 CA COPYRIGHT 2002 ACS  
AN 129:193625 CA  
TI Considerations on the potentiometric log P determination  
AU Kramer, Stefanie D.; Gautier, Jean-Claude; Saudemon, Philippe  
CS Pharmaceutical Sciences Department. Sanofi Recherche, Montpellier, Fr.  
SO Pharmaceutical Research (1998), 15(8), 1310-1313  
AB A complementary approach to the existing calcn. program to calc. log P values from the titrated aq. pKa and the apparent pKa values (pKaapp) in biphasic systems. The presented data anal. method can be used for all kinds of protonable and deprotonable mols. like monoprotic and multiprotic acids and bases, mixed functional, and zwitterion forming compds. It permits an accurate evaluation of the results, which is not always evident when using the complex calcn. program delivered with the instruments.

L28 ANSWER 61 OF 256 CA COPYRIGHT 2002 ACS  
AN 126:270592 CA  
TI The structure of mesophases of binary and multicomponent mixtures of some cholesteric liquid crystals  
AU Obadovic, Dusanka Z.; Vajda, Aniko; Katona, Tibor Toth; Marinkovic - Neducin, Radmila  
CS Institute of Physics, Faculty of Sciences, Novi Sad, Yugoslavia  
SO Molecular Crystals and Liquid Crystals Science and Technology, Section A: Molecular Crystals and Liquid Crystals (1995), 265 (Proceedings of the 15th

AB International Liquid Crystal Conference, 1994, Pt. 5), 2701-2707  
Binary and **multicomponent mixts.** of cholesteryl enanthate with cholesteryl nonanoate and cholesteryl formate were studied. The aim of the study is the prepn. of the system with phase transition **temp.** close to room **temp.** Phase **diagrams** of binary **mixts.** are **formed** from data obtained by the optical microscopy and DS calorimetry and the shift of phase transition points of order 30-50° with respect to initial components was established. In the case of three- and four-component mixts., the presence of enantiomorphic phase transitions of smectic and cholesteric type, resp. was identified. X-ray diffraction data have enabled the characterization of the structure of smectic or cholesteric mesophase and the calcn. of mol. parameters: apparent length of the mols. l and the av. intermol. distance (D).

L28 ANSWER 66 OF 256 CA COPYRIGHT 2002 ACS

AN 126:214574 CA

TI Modeling of the solubility of a one-component H<sub>2</sub>O or CO<sub>2</sub> fluid in silicate liquids

AU Papale, Paolo

CS Cent. Studio Geos logia Strutturale Dinamica Appennino, Pisa, I-56126, Italy

SO Contributions to Mineralogy and Petrology (1997), 126(3), 237-251

AB The modeling of the solv. of **water** and carbon dioxide in silicate **liqs.** (flash problem) is performed by assuming mech., thermal, and chem. equil. between the **liq.** magma and the gas phase. The **liq.** phase is treated as a **mixt.** of ten silicate components + H<sub>2</sub>O or CO<sub>2</sub>, and the gas phase as a pure H<sub>2</sub>O or CO<sub>2</sub>. A general model for the solv. of a volatile component in a **liq.** is adopted. This requires the definition of a **mixing** equation for the excess Gibbs free energy of the **liq.** phase and an appropriate ref. state for the dissolved volatile. To constrain the model parameters and identify the most appropriate form of the solv. equations for each dissolved volatile, a large no. of exptl. solv. detns. (640 for H<sub>2</sub>O and 263 for CO<sub>2</sub>) have been used. These detns. cover a large region of the P-T-compn. space of interest. The resultant **water** and carbon dioxide solv. models differ in that the **water** model is regular and isometric, and the carbon dioxide model is regular and non-isometric. This difference is consistent with the different speciation modalities of the two volatiles in the silicate **liqs.**, producing a compn.-independent partial molar volume of dissolved **water** and a compn.-dependent partial molar volume of dissolved carbon dioxide. The H<sub>2</sub>O solv. model may be applied to natural magmas of virtually any compn. in the P-T range 0.1 MPa-1 GPa and > 1000 K, whereas the CO<sub>2</sub> solv. model may be applied to several GPa pressures. The general consistency of the **water** solv. data and their relatively large no. as compared to the **calibrated** model parameters (11) contrast with the large inconsistencies of the carbon dioxide solv. detns. and their low no. with respect to the CO<sub>2</sub> model parameters (22). As a result, most of the solv. data in the **database** are reproduced within 10% of approxn. in the case of **water**, and 30% in the case of carbon dioxide. When compared with the exptl. data, the H<sub>2</sub>O and CO<sub>2</sub> solv. models correctly predict many features of the satn. surface in the P-T-compn. space, including the change from retrograde to prograde H<sub>2</sub>O solv. in albitic **liqs.** with increasing pressure, the so-called alkali effect, the increasing CO<sub>2</sub> solv. with increasing degree of silica undersatn., the Henrian behavior of CO<sub>2</sub> in most silicate **liqs.** up to about 30-50 MPa, and the proportionality between the fugacity in the gas phase, or the satn. activity in the **liq.** phase, and the square of the mole fraction of the dissolved volatile found in some unrelated silicate **liq.** compns.

L28 ANSWER 89 OF 256 CA COPYRIGHT 2002 ACS

AN 124:218999 CA  
TI A simple method for the titration of multicomponent acid-base mixtures  
AU Toisio, T.; Heikonen, M.  
CS Valio Ltd., Helsinki, FIN-00370, Finland  
SO Fresenius' Journal of Analytical Chemistry (1996), 354(3), 271-7  
AB A titrn. method was developed to analyze acid mixts., in which the pK values differed by 0.5 to 1 pH units. Instead of the use of equivalence points a buffer capacity curve is numerically derived from the titrn. curve resulting in a presentation similar to chromatograms and spectra. The consumption of the NaOH titrant is detd. within pH intervals of 0.2-0.6 units around the pK values of the components. The buffer capacity measured is expressed as the consumption of NaOH over the pH interval. The amts. of compds. are found from these results using simple models of chemometrics. The method was applied to a mixt. of formic and acetic acids with concns. of 0-3 mmol/20 mL with an error of 0-0.05 mmol. Also a curve-fitting method based on a theor. equation of buffer capacity can be applied with an error slightly larger than with the previous method. In this case, the pK values were also computed. For titrns. beyond the pH range 4-10, the buffer capacity of H<sub>2</sub>O has to be subtracted from the titrn. results. The whole procedure requires including the computations ~3-6 min.

L28 ANSWER 93 OF 256 CA COPYRIGHT 2002 ACS

AN 124:157363 CA  
TI Thermodynamics of aqueous electrolytes at high temperatures by the isopiestic technique  
AU Holmes, H. F.; Mesmer, R. E.  
CS Chemical and Analytical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN, 37831-6110, USA  
SO Physical Chemistry of Aqueous Systems: Meeting the Needs of Industry, Proceedings of the International Conference on the Properties of Water and Steam, 12th, Orlando, Fla., Sept. 11-16, 1994 (1995), Meeting Date 1994, 533-40. Editor(s): White, Howard J., Jr. Publisher: Begell House, New York, N. Y.  
AB Excess thermodn. properties of a wide variety of aq. electrolyte solns. at elevated temps. were detd. with the ORNL high-temp. isopiestic facility. This unique exptl. app. provides very precise results over the useful temp. range of 110-250°. The isopiestic method is a comparative technique which, in the present case, uses the Pitzer-Peiper-Busey formulation for NaCl(aq) as the ref. electrolyte. At elevated temps. the ion-interaction model of Pitzer continues to be the most useful description of the exptl. results. The exptl. program included the alkali metal chlorides, sulfates, hydroxides, bromides, and bisulfates, the alk. earth metal chlorides, and several specific compds. of scientific and practical interest. Numerous common-ion mixed electrolyte solns. were also investigated in this program. In general, the activity coeffs. of all the studied electrolytes decrease with increasing temp. However, prominent differences between members of the same family remain, particularly when considered as the excess Gibbs free energy. The tendency for ion assocn. increases with increasing temp. and becomes a factor at the higher temps. Trends and specific effects are illustrated with examples taken from the database generated in our high-temp. thermodn. program.

L28 ANSWER 108 OF 256 CA COPYRIGHT 2002 ACS

AN 122:70730 CA  
TI Qualitative analysis in the near-infrared region  
AU Downey, Gerard  
CS Dep. Plant Marine Foods, Natl. Food Cent., Dublin, UK  
SO Analyst (Cambridge, United Kingdom) (1994), 119(11), 2367-75

AB A review, with 29 refs., provides an up-to-date overview of the chemometric approaches available to users of near-IR spectroscopy specifically for the soln. of qual. anal. problems. The problems addressed include discrimination between similar materials of different functional classes; identification of pure chems. using a previously established spectra library; selection of optimum calibration sample sets with detection of outlying and redundant samples; and preliminary studies into the anal. of mixts. Among procedures discussed are discriminant methods (both supervised and unsupervised) and pattern recognition techniques.

L28

ANSWER 152 OF 256 CA COPYRIGHT 2002 ACS

AN 115:84579 CA

TI Experimental methods for determining the eutectic composition of a multi-component liquid crystal mixture

AU Margerum, J. David; Van Ast, Camille I.; Myer, Gary D.; Smith, Willis H., Jr.

CS Hughes Res. Lab., Malibu, CA, 90265, USA

SO Molecular Crystals and Liquid Crystals (1991), 198, 29-36

AB Exptl. techniques are described for detg. the eutectic compn. of multicomponent mixts. of nematic liq. crystals. These techniques were applied to the formulation of nematic esters, when the idealized eutectic compn. calcd. by the Schroeder-Van Laar relationship did not give a good m.p. min. for the mixt. One exptl. procedure was based on the assumption that the compn. of the initial nematic melt from a frozen, crystd. mixt. is closer to a true eutectic than is the calcd. value from which the frozen mixt. was formulated. Another exptl. procedure was based on the assumption that a new eutectic could be obtained by adding small amts. of a new component to an existing multi-component eutectic mixt., using the plot of the m.p. vs. the percentage of the new component added to det. a new eutectic mixt. corresponding to a new m.p. min. High performance liq. chromatog. was used to est. the purity of each component, and to analyze quant. the component compn. of each melt. The calibration plots for each liq. crystal component, as well as the chromatog. anal. of the mixts. are shown.

AB5

L28

ANSWER 169 OF 256 CA COPYRIGHT 2002 ACS

AN 111:239373 CA

TI Calorimetric determination of mixing energies in multicompartiment systems. Part 1: Construction of a titration calorimeter and interpretation by means of the deconvolution of the measuring function

AU Mueller, B. W.; Franzky, H. J.

CS Christian-Albrechts Univ., Kiel, Fed. Rep. Ger.

SO Pharmazie (1989), 44(7), 462-6

LA German

AB Microemulsions (esp. pharmaceutical) contg. surfactants, cosurfactants, oil, and water form oil-in-water and water-in-oil emulsions if they are dispersed systems and not colloidal solns. The study deals with the construction of a titrn. calorimeter and detn. of mixing enthalpies of a 2-component system by means of the deconvolution of the measuring function. A detailed scheme for the calorimeter construction, its calibration aspects and free mixing enthalpy of ethoxylated glycerol monostearate-H<sub>2</sub>O systems are discussed.

=> log y

STN INTERNATIONAL LOGOFF AT 07:05:10 ON 25 NOV 2002

=> d his

(FILE 'HOME' ENTERED AT 13:24:35 ON 25 NOV 2002)

FILE 'CA' ENTERED AT 13:24:44 ON 25 NOV 2002

L1 36849 S (ADD? OR INJECT?) (2A) (AMOUNTS OR PORTIONS OR VOLUMES) OR (MULTIPLE OR  
SEVERAL OR PLURAL?) (3A) (ADDITIONS OR INJECTIONS)  
L2 18454 S L1 AND (MIXTURE OR MIXED OR MIXING OR MIX OR SOLUTION)  
L3 694 S ((ADD? OR INJECT?) (2A) (AMOUNTS OR PORTIONS OR VOLUMES) OR (MULTIPLE OR  
SEVERAL OR PLURAL?) (3A) (ADDITIONS OR INJECTIONS)) /TI, ST, IT  
L4 167 S L2 AND L3  
L5 55 S L4 AND (PROPERTY OR STEPWISE OR STEP WISE)  
L6 112 S L4 NOT L5  
L7 4 S L6 AND (CHCL3 OR STANDARD ADDITION OR REFRACTIVE INDEX)  
L8 168 S L1 AND (STEPWISE OR STEP WISE OR GRADIENT OR STANDARD) (2A) (ADDITION  
OR INJECTION)  
L9 72 S L8 AND (CALIBRAT? OR PARALLEL OR TITRANT OR TITRAT? OR (ELECTRODE OR  
CONCENTRAT? OR HANDLING) /TI)  
L10 121 S L5, L7, L9  
L11 106 S L10 NOT PY>1998

=> d bib, ab 1-106 111

L11 ANSWER 2 OF 106 CA COPYRIGHT 2002 ACS

AN 128:123233 CA

TI Asymmetric distribution of results in **calibration** curve and **standard addition** evaluations

AU Renman, Lars; Jagner, Daniel

CS Analytical and Marine Chemistry, Department of Chemistry, University of Goteborg, S-412 96 Goteborg, Swed.

SO Analytica Chimica Acta (1997), 357(1-2), 157-166

AB The inherent asymmetry in the application of linear regression anal. to the detn. of sample analyte concns. using **calibration** curve or **std. addn.** evaluations gives rise to systematic errors. On the av., this always results in an overestimation of the true analyte concns. in **std. addn.** evaluations, while in **calibration** curve evaluations, the mean relative error depends on the value of sample concn. in relation to the analyte concns. used for the **calibration** curve. In both evaluation techniques, the distribution of the results will deviate from a Gaussian distribution even if all anal. signals are normally distributed. It is shown that, for the **std. addn.** technique and for samples with low analyte concns. evaluated by the **calibration** curve technique, optimum precision and accuracy is obtained by using a min. no. of **calibration** points or **std. addns.**, and performing **multiple** measurements on these. It is also shown that the linear regression correlation coeff. is a very poor indicator of the accuracy and precision in multiple-point **std. addn.** evaluations. Weighted linear regression can be used to decrease the magnitudes of the systematic errors, but due to the inherent asymmetry, the distribution of the results will nevertheless be non-Gaussian. A publically available, inhouse constructed Windows 3.1/Windows 95 program, capable of simulating all kinds of **calibration** curve and **std. addn.** evaluations, was used for all calcns.

L11 ANSWER 6 OF 106 CA COPYRIGHT 2002 ACS

AN 123:51462 CA

TI Determination of zinc in plasma by atomic absorption spectrometry with a graphite furnace and pyrolytic platform

AU Burrini, C.; Borghi, G.; Fuzzi, G.

CS Ist. Ricerche Clin., Florence, Italy

SO Giornale Italiano di Chimica Clinica (1994), 19(2), 127-31

AB We present a precise and accurate method for the detn. of zinc in blood

plasma by at. absorption spectrometry with graphite furnace and pyrolytic platform. The samples were dild. 40-fold with a 0.1% nitric acid and 0.025% Triton X 100 soln., six microliters of this diln. were utilized for the measurement. Zinc concns. were calcd. by comparison with a calibration curve prep'd. by adding known amts. of a std. soln. to a dild. sample (std. addns. technique). The detection limit was 0.03 mg/L. Within-run CVs were 1.30% and 2.00% for plasma zinc concns. of 0.76 and 1.57 mg/L, while between-run CV was 3.86% for a concn. of 0.86 mg/L.

L11 ANSWER 8 OF 106 CA COPYRIGHT 2002 ACS  
AN 122:280756 CA  
TI Validation of an analytical instrumental method by standard addition methodology  
AU Rodriguez, Luis Cuadros; Campana, Ana M. Garcia; Barrero, Fermin Ales; Linares, Carlos Jimenez; Ceba, Manuel Roman  
CS Fac. Sci., Univ. Granada, Granada, 18071, Spain  
SO Journal of AOAC International (1995), 78(2), 471-6  
AB A statistical procedure to validate an anal. methodol. by std. addn. methodol. is described. The data set obtained in 3 calibration expts. with std. dilns., std. addns., and portions of sample was used. The accuracy of the anal. results is checked by comparison of analyte contents in the different calibrations and from the recovery. Math. expressions to est. the statistical parameters are proposed. The statistical protocol was applied to fluorometric detn. of Mo with alizarin S in vegetable tissues.

L11 ANSWER 19 OF 106 CA COPYRIGHT 2002 ACS  
AN 115:196939 CA  
TI In situ measurement of electrode slope and gravimetric multiple standard addition analysis by ion selective potentiometry without prior calibration of electrode  
AU Chaudhuri, N. K.; Sawant, R. M.  
CS Fuel Chem. Div., Bhabha At. Res. Cent., Bombay, 400 085, India  
SO Analytical Letters (1991), 24(9), 1605-24  
AB Two methods of calcn. for the detn. of an unknown concn. by gravimetric multiple std. addn. anal. using ion selective potentiometry without prior calibration of the electrode are described. These are based on simple calcn. procedures involving linear least square fitting to Gran's equation to evaluate first the actual electrode slope 'in situ', then the unknown concn. and the cell const. One method is iterative and the other is noniterative. The applicability of the methods is demonstrated by processing the exptl. data obtained by using fluoride and uranyl ion selective electrodes.

L11 ANSWER 24 OF 106 CA COPYRIGHT 2002 ACS  
AN 114:74518 CA  
TI Linearized multiple standard additions for the potentiometric determination of weak acids  
AU Macca, Carlo  
CS Dep. Inorg., Organomet. Anal. Chem., Univ. Padova, Padua, I-35131, Italy  
SO Talanta (1990), 37(12), 1141-9  
AB The feasibility of potentiometric detn. of weak monoprotic acids by the multiple std. addn. method is examd. A std. soln. of pure weak acid is added to the soln. contg. an unknown amt. of the same weak acid, alone or mixed with its conjugate base. The exptl. data are processed by Gran-type plots, for which rigorous and approx. equations are obtained. It is shown that weak acids can be detd. by multiple std. addns. with a precision comparable with that of the usual kinds of potentiometric

addn. methods. The validity range of the approx. equations is established. Linear equations similar to those of Hofstee, Scatchard, Lineweaver and Burk, and Scott are also obtained, by which acidity consts. can be detd. together with equivalence vols. The effects of systematic and random measurement errors are examd.

L11 ANSWER 25 OF 106 CA COPYRIGHT 2002 ACS

AN 113:144237 CA

TI Preparation of solutions before titration by the standard addition technique

AU Zhukov, B. D.

CS Pac. Inst. Oceanol., Vladivostok, USSR

SO Zhurnal Analiticheskoi Khimii (1990), 45(6), 1167-72

AB A method is described for prep. solns. for titrn. by the std. addn. method involving the soln. to be titrated and the titrant and including the distribution of the sample between them. Tests showed the effectiveness of such a prepn. on an example of ionometry during the development of conditions providing for minimal consumption of the indifferent electrolyte salt, independent of the vol. and the no. of addns. of such anal. characteristics as the compn. of the supporting electrolyte, the ionic strength, the slope of the electrode function, etc. In an example of detg. the F- concn. in aq. solns. by using the multiple std. addns. method with ion-selective electrodes, the equalization of the compns. and the value of the physicochem. characteristics of the soln. being titrated and the titrant also allow one to eliminate the influence of effects related to diln. of the soln. being titrated.

L11 ANSWER 27 OF 106 CA COPYRIGHT 2002 ACS

AN 112:110981 CA

TI Hybrid multiple standard additions-analyte addition method for ion-selective electrodes with integral calibration

AU Velinov, G.; Panushev, A.

CS Med. Acad., Sofia, 1000, Bulg.

SO Analyst (Cambridge, United Kingdom) (1989), 114(8), 929-32

AB A hybrid multiple std. addns.-analyte addn. method for ion-selective electrodes is described in which the calibration of the potentiometric cell and the detn. of the unknown concn. of the sample are carried out in a single expt. This ensures max. constancy of the calibration characteristics,  $E^\circ$  and S, of the cell. The proposed method allows the detn. of trace amts. (100  $\mu$ g) of an analyte. The data treatment includes an iterative minimization procedure using the least-squares sum method, which improves the accuracy and the statistical reproducibility of the results. The method can be automated by means of an automatic titrator, controlled by an HP-85B microcomputer. A BASIC program was constructed for this purpose. The method was tested by applying it to the detn. of sodium, potassium, chloride and fluoride ions and the errors of the results were less than 1%. The detn. limit of the method was investigated by detg. decreasing concns. of fluoride ions. It was found that the method gives satisfactory results over the entire linear range of the ion-selective electrode.

L11 ANSWER 29 OF 106 CA COPYRIGHT 2002 ACS

AN 108:215482 CA

TI Method of parallel addition in ionometry

AU Urusov, Yu. I.; Tsygankov, A. M.; Zhukov, A. F.; Firer, A. A.

CS Moscow Chemicotechnol. Inst., Moscow, USSR

SO Zhurnal Analiticheskoi Khimii (1988), 43(3), 421-5

AB A new method for detg. anions in acid media is based on addn. of equal

vols. of a std. soln. with different analyte concns. to 2 parallel samples of equal vols. The effect of detn. conditions on the relative error has been examd. by taking  $\text{AuCl}_4^-$  and  $\text{PtCl}_6^{2-}$  as examples. The method is useful for the detn. of anions in solns. of different acid concn. by potentiometry with ion-selective electrodes.

L11 ANSWER 46 OF 106 CA COPYRIGHT 2002 ACS

AN 100:25847 CA

TI Automatic titration by stepwise addition of equal volumes of titrant. Part VIII. Determination of alkalinity and total carbonate in seawater

AU Johansson, Axel; Johansson, Sten; Gran, Gunnar

CS Dep. Anal. Chem., R. Inst. Technol., Stockholm, S-100 44, Swed.

SO Analyst (Cambridge, United Kingdom) (1983), 108(1290), 1086-90

AB The reliability of a set of linear equations for the evaluation of titrn. data was investigated for the detn. of alky. and total  $\text{CO}_3^{2-}$  in seawater by potentiometric titrn. with std. HCl soln. The method requires that polyprotic acids be treated as a mixt. of monoprotic acids and approx. values for equil. consts. for the acid-base pairs is known. The results agreed well with those obtained by nonlinear curve-fitting methods.

L11 ANSWER 54 OF 106 CA COPYRIGHT 2002 ACS

AN 94:202069 CA

TI Automatic titration by stepwise addition of equal volumes of titrant. Part VI. Further extension of the Gran I method for calculation of the equivalence volume in acid-base titrations

AU Gran, Gunnar; Johansson, Axel

CS Dep. Anal. Chem., R. Inst. Technol., Stockholm, S-10044/70, Swed.

SO Analyst (London) (1981), 106(1259), 231-42

AB The equivalence vol.,  $V_e$ , was calcd. from titrn. data by a method of stepwise addn. of equal vol. of titrant combined with an extended version of the Gran I method. The method can be used for monoprotic acids with  $\log K \leq 10$ . The  $V_e$  values for most di- and triprotic acids can also be calcd. by this method.

L11 ANSWER 56 OF 106 CA COPYRIGHT 2002 ACS

AN 93:211078 CA

TI Automatic titration by stepwise addition of equal volumes of titrant. Part V. Extension of the Gran I method for calculation of the equivalence volume in acid-base titrations

AU Johansson, Axel; Gran, Gunnar

CS Dep. Anal. Chem., R. Inst. Technol., Stockholm, 10044/70, Swed.

SO Analyst (London) (1980), 105(1253), 802-10

AB The equiv. vol. is calcd. from titrn. data by a simple method based on stepwise addn. of equal vols. of titrant combined with an extension of the Gran I method. This method is also used to det. the conditional normal potential and the const. in the junction potential for an electrode couple in a given medium. Titrns. of very weak acids can not be evaluated by this method.

L11 ANSWER 58 OF 106 CA COPYRIGHT 2002 ACS

AN 92:33272 CA

TI High accuracy titrimetric analysis

AU Spivakovskii, V. B.; Dovgopol, O. S.; Makovskaya, G. V.; Moisa, L. P.

CS Inst. Met. Phys., Kiev, USSR

SO Zh. Anal. Khim. (1979), 34(9), 1681-6

AB A method for the detection of the deviation of the titrn. end point from

the equivalence point and for taking into account coordination of all anal. operations from the viewpoint of accuracy ensures high accuracy in the titrimetric detns. of macroconcns. of elements or the main components of substances to be analyzed. The method was tested on the titrimetric detn. of Pb in Pb(NO<sub>3</sub>)<sub>2</sub> of spectral purity with Complexon III at pH 4-8. The method involves several std. addns. of Pb, measurement of the a.c. polarog. peak current of Pb after each addn., and extrapolation of the curve obtained from these measurements.

- L11 ANSWER 60 OF 106 CA COPYRIGHT 2002 ACS  
AN 91:199756 CA  
TI Automatic titration by stepwise addition of equal volumes of titrant. Part IV. General-purpose program for evaluating potentiometric acid-base titrations  
AU Johansson, Axel; Johansson, Sten  
CS Dep. Anal. Chem., R. Inst. Technol., Stockholm, S-100 44/70, Swed.  
SO Analyst (London) (1979), 104(1240), 601-12  
AB A computer program, TITRA, for evaluating acid-base titrn. results, using nonlinear regression techniques, was studied. All n-protic acids were treated as a mixt. of n monoprotic acids of the same molality as the n-protic acid. The parameter calcns. were performed in an appropriate sequence. No preliminary ests. of the required concns. were necessary. The method was applied to samples of mono- and polyprotic acids, mixts. of acids, ampholytes, salts of weak acids, acids with an abnormal sequence of stability const. values, and bases. E.g., for a mixt. of HCl, phthalic acid, and barbital, the amts. found were 1.000, 0.9992 and 1.0055 mmol, resp., compared with 1.000, 1.0025 and 1.0011 mmol added, giving a recovery of 100.0, 99.7 and 100.4%, resp.
- L11 ANSWER 61 OF 106 CA COPYRIGHT 2002 ACS  
AN 90:214572 CA  
TI Microcomputer-aided high-speed potentiometric titration system by linear titration plots  
AU Yamaguchi, Shinichiro; Kusuyama, Takashi  
CS Wakayama Res. Lab., Kao Soap Co., Ltd., Wakayama, Japan  
SO Fresenius' Z. Anal. Chem. (1979), 295(4), 256-9  
AB An app. for high-speed potentiometric titrn. was assembled and its advantage was demonstrated. Titrant addns. were made stepwise in large vols. The optimum increment vols. were automatically chosen by microcomputer, depending upon the sample concn. Time intervals between the successive addns. were controlled so as to add a new increment immediately after the electrode was equilibrated. On-line calcn. of the equivalence vol. was conducted based upon linear titrn. plots by using only 4 titrn. points before the equivalence point. The app. was capable of detg. the concn. of strong and weak monoprotic acids in <22 s with relative std. deviations of 0.1-0.2%.
- L11 ANSWER 62 OF 106 CA COPYRIGHT 2002 ACS  
AN 89:172898 CA  
TI Automatic titration by stepwise addition of equal volumes of titrant. Part III. Use of linear equations to calculate equivalence volumes in acid-base titrations  
AU Johansson, Axel; Johansson, Sten  
CS Dep. Anal. Chem., R. Inst. Technol., Stockholm, Swed.  
SO Analyst (London) (1978), 103(1225), 305-16  
AB A computational procedure is described for calcg. equivalence vols. for the titrn. of monoprotic acids, bases, and ampholytes with log K (K = stability const.) ≤ 11. The procedure is based on the soln. of a

set of linear equations and requires only a few sets of measurements of emf. vs. titrant vol. plus the initial vol. and titrant concn. Log K values are not required and emf. measurements may have a const. systematic error of  $\pm 6$  meV, corresponding to  $\pm 0.1$  pH unit. The program can automatically select appropriate measurements. Exptl. results had std. deviations  $< 0.2\%$ .

L11 ANSWER 66 OF 106 CA COPYRIGHT 2002 ACS

AN 87:77978 CA

TI Acid-base titrations by stepwise addition of equal volumes of titrant with special reference to automatic titrations. IV.

Photometric titration of an acid

AU Pehrsson, Lennart; Ingman, Folke

CS Dep. Anal. Chem., R. Inst. Technol., Stockholm, Swed.

SO Talanta (1977), 24(2), 87-90

AB The method of stepwise addn. of titrant in acid-base titrns.

(1977) is applied to photometric titrn. of monoprotic acids. The highest precision is obtained when the absorbance of the titrn. mixt. changes linearly with each addn. of titrant. For weak acids good results are found if the stability consts. of the acid and indicator differ by 0.3-0.5 logarithmic units. The method is tested on the titrn. of 0.01006M HCO<sub>2</sub>H with 0.1M NaOH and bromophenol blue indicator. Ten consecutive titrns. gave the concn. as 0.01007M with a coeff. of variation 0.12%. The advantages and disadvantages of the method are discussed.

L11 ANSWER 67 OF 106 CA COPYRIGHT 2002 ACS

AN 87:77942 CA

TI Acid-base titrations by stepwise addition of equal volumes of titrant with special reference to automatic titrations. III.

Presentation of a full automatic titration apparatus and of results supporting the theories given in the preceding parts

AU Pehrsson, Lennart; Ingman, Folke

CS R. Inst. Technol., Stockholm, Swed.

SO Talanta (1977), 24(2), 79-85

AB The title app. holds 200 sample tubes and performs the following operations; pipetting of sample and addn. of neutral salt to give const., high ionic strength; thermostatic temp. control to  $25 \pm 0.1^\circ$ ; addn. of titrant in equal vols. and detn. of the electrode potential after each addn.; rinsing of titrn. vessel and electrode couple; sample changeover. Titrn. results for monoprotic acids, e.g. HCO<sub>2</sub>H, HCO<sub>2</sub>H-EtCO<sub>2</sub>H mixts., tartaric acid, K H phthalate, and HCO<sub>2</sub>H-HCO<sub>2</sub>-mixts. are given. These titrns. cannot be evaluated by the methods of G. Gran (1952) and B. H. J. Hofstee (1960) but the proposed method (1976) gives results accurate to 0.1%. The method is better than common titrn. methods in that all the data are used in the evaluation, permitting a statistical treatment.

L11 ANSWER 68 OF 106 CA COPYRIGHT 2002 ACS

AN 86:182361 CA

TI Acid-base titrations by stepwise addition of equal volumes of titrant with special reference to automatic titrations. II. Theory of titration of mixtures of acids, polyprotic acids, acids in mixture with weak bases, and ampholytes

AU Pehrsson, Lennart; Ingman, Folke; Johansson, Sten

CS R. Inst. Technol., Stockholm, Swed.

SO Talanta (1976), 23(11-12), 781-8

AB A general method is given for evaluating titrn. data for mixts. of

acids, and for acids **mixed** with weak bases, which allows use of relative H concn. data, thus requiring only an approx. **calibration** of the electrode system. For simple systems, only a rough calcn. of stability const. is required. Detailed example calcns. are given for **titrating** a binary acid **mixt.**, a diprotic acid, an acid-conjugate base system, and an ampholyte.

L11 ANSWER 69 OF 106 CA COPYRIGHT 2002 ACS  
AN 86:8518 CA  
TI Determination of lead in saline water under use of flameless atomic-adsorption spectrophotometry  
AU Kussmaul, H.; Majlis, S. K.  
CS Frankfurt/Main, Ger.  
SO Gas- Wasserfach, Wasser - Abwasser (1975), 116(12), 552-4  
LA German  
AB While estg. Pb in the water samples by means of the flameless atomic absorption spectrophotometry (graphite-pipe curvette), disturbances depending on the matrix compn. were obsd. It was evident that these were caused mainly by the Na in the surface waters. Other ions could cause signal depression or intensification. For elimination of these disturbances, an addnl. procedure was suggested, in which the **calibration** curve was plotted in a soln. with the same matrix compn. as that of the measuring soln. It occurred in this case by gradual **addn.** of the **std.** soln. to the water sample. A water sample 100 ml is acidified with concd. H<sub>2</sub>SO<sub>4</sub> 1 ml, known Pb **amts.** are **added** stepwise, and the respective extinction coeffs. are measured. By this the necessity of a correction of the extinction depression was omitted, as the addn. procedure was equiv. to the plotting of the **calibration** curve of a soln. which contained the same matrix as the test sample.

L11 ANSWER 70 OF 106 CA COPYRIGHT 2002 ACS  
AN 85:186166 CA  
TI Automated computer-controlled solution **handling** system utilizing weights of solution  
AU Renoe, B. W.; O'Keefe, K. R.; Malmstadt, H. V.  
CS Sch. Chem. Sci., Univ. Illinois, Urbana, Ill., USA  
SO Anal. Chem. (1976), 48(4), 661-6  
AB An automated sample and reagent soln. prepn. system, which is generally applicable in the anal. lab., was designed and tested. The new system utilizes an electronic sensor to weigh accurately the nominal aliquots of sample and reagent solns. that are added to a disposable beaker. Each plastic beaker on a turntable is automatically positioned on the wt. sensor. Reagent and sample solns. are added by gravity feed for selected time/ intervals to provide nominal amts. Each reagent or sample is accurately weighed after addn., and the beaker is then automatically moved to a stirring station while another beaker is moved into position for wt. measurements. The **amts.** of reagents **added** to the beaker can be incrementally adjusted as desired. The operational modes are specified by interaction through FORTRAN programming and FORTRAN callable subroutines, which control or accumulate data concerning the system turntable, wt. sensor, soln. delivery devices and mixer, and the computer peripherals. The anal. utility of the system is demonstrated by data obtained in automated prepn. of working curves and **std.-addn.** procedures.

L11 ANSWER 73 OF 106 CA COPYRIGHT 2002 ACS  
AN 79:73155 CA  
TI Automated system for photometric titration by stepwise addition of equal **volumes** of titrant

AU Pehrsson, Lennart; Johansson, Axel  
CS Dep. Anal. Chem., R. Inst. Technol., Stockholm, Swed.  
SO Anal. Chim. Acta (1973), 66(1), 67-74  
AB A completely automatic system for photometric titrns. delivers measured vols. of sample, indicator soln., and buffer soln., titrates, and finally rinses the titrn. vessels. Titrns. are performed by adding the titrant stepwise in equal vols. to the sample, measuring the absorbance after each addn., and calcg. the equivalence vols. The system performs ~30 titrns./hr and has a loading capacity of 200 samples. It was tested by titrating Ca with EGTA in presence of calmagite as indicator.

L11 ANSWER 81 OF 106 CA COPYRIGHT 2002 ACS  
AN 73:126566 CA  
TI Automatic titration by stepwise addition of equal volumes of titrant. II. Automatic titration system  
AU Johansson, Axel; Pehrsson, Lennart.  
CS Dep. Anal. Chem., Roy. Inst. Technol., Stockholm, Swed.  
SO Analyst (London) (1970), 95(1132), 652-6  
AB An automatic potentiometric titrn. app. pipets, dils., and titrates (by addn. of equal vols. of titrant) the sample and washes the electrodes and titrn. vessels, at a rate of ≤30 samples/hr. HCl (0.03354M) and 0.02293M HOAc in a binary mixt. were detd. by using the app. with + 0.00016M and -0.00017M abs. errors, resp., and with 0.2 and 0.9% relative std. deviations, resp.

L11 ANSWER 82 OF 106 CA COPYRIGHT 2002 ACS  
AN 73:83501 CA  
TI Computer approach to ion-selective electrode potentiometry by standard addition methods  
AU Brand, Michael J. D.; Rechnitz, Garry A.  
CS Dep. of Chem., State Univ. of New York, Buffalo, N. Y., USA  
SO Anal. Chem. (1970), 42(11), 1172-7  
AB Methods are described for detg. an unknown concn. by using an ion-selective electrode without prior calibration of the electrode. The methods are based on std. addn. procedures. In the simplest case, only 2 std. addns. are required and a simple calcn. is described which can be performed by a computing calculator. To obtain high accuracy in the detn. of unknown concns., multiple addns. are made and a least squares curve fitting method is used to evaluate the unknown concn., electrode slope, and std. potential. A computer program to accomplish this calcn., ADDFIT, is given in Fortran IV. The effectiveness of these methods is demonstrated by expts. on Pb and chloride samples.

L11 ANSWER 83 OF 106 CA COPYRIGHT 2002 ACS  
AN 73:51898 CA  
TI Automatic titration by stepwise addition of equal volumes of titrant. I. Basic principles  
AU Johansson, Axel  
CS Roy. Inst. Technol., Stockholm, Swed.  
SO Analyst (London) (1970), 95(1131), 535-40  
AB The basic principles of a potentiometric titrn. method, which is based on making potential measurements after each addn. of titrant in equal-vol. increments, are described. The method is esp. suitable for automation, e.g. in biochem. and process control anal. The method is demonstrated by NaOH titrns. of HCl and HOAc, both alone and in mixts.

L11 ANSWER 91 OF 106 CA COPYRIGHT 2002 ACS

AN 64:30996 CA

OREF 64:5759f-h

TI Phase titrations. V. Nitroalkanes. Improving the phase-titration end point

AU Rogers, D. W.; Lillian, D.; Chawla, I. D.

CS Am. School, Madrid

SO Talanta (1966), 13(2), 313-18

AB cf. CA 62, 12648f. End points for direct phase titrns. of binary solns. of nitropropanes in H<sub>2</sub>O-miscible solvents are fair and, because of the steepness of the calibration curve, results are adequate. EtNO<sub>2</sub> ethane, in binary combination, gives poor end points but, over part of the optimum titrn. range, results are good. MeNO<sub>2</sub> gives end points which are almost useless. Addn. of standard amts. of PhNO<sub>2</sub>, which gives excellent phase-titrn. end points, improves the composite MeNO<sub>2</sub>-PhNO<sub>2</sub>-H<sub>2</sub>O-miscible component end point markedly. Because the PhNO<sub>2</sub> concn. is const., the H<sub>2</sub>O titer is a function only of the MeNO<sub>2</sub> concn. Addn. of const. amts. of PhNO<sub>2</sub> also increases the optimum titrn. range. Results given for all systems arc comparable in accuracy with systems previously reported which are favorable to direct phase titrn.

=> log y

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